2,3,4,6,9-pentachlorodibenzofuran

Other names: Dibenzofuran, 2,3,4,6,9-pentachloro
Inchi: InChI=1S/C12H3Cl5O/c13-5-1-2-6(14)12-8(5)4-3-7(15)9(16)10(17)11(4)18-12/h1-3H
InchiKey: VANGHZRYKXDPRR-UHFFFAOYSA-N
Formula: C12H3Cl5O
SMILES: Clc1cc2c(oc3c(Cl)ccc(Cl)c32)c(Cl)c1Cl
Mol. weight [g/mol]: 340.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.24		Crippen Method
logp	6.853		Crippen Method
mcvol	188.630	ml/mol	McGowan Method
rinpol	2511.00		NIST Webbook
rinpol	2476.00		NIST Webbook
rinpol	2482.00		NIST Webbook
rinpol	2476.00		NIST Webbook
rinpol	2511.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R29720&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices